

14-December-2001**ROBUST SUMMARY FOR 1,5,9-CYCLODODECATRIENE**Summary

1,5,9-Cyclododecatriene is a liquid with a yellow tint and pungent odor. It has a melting point of -17°C and boiling point of 237°C. 1,5,9-Cyclododecatriene has an autoignition temperature of 244°C, flash point of ca. 88°C, water solubility of 5 mg/L at 20°C, and vapor pressure of 0.09 mm Hg.

Fugacity model predicts that 1,5,9-cyclododecatriene (CDDT) will remain predominately in the air compartment and is expected to exist almost entirely in the vapor phase. The rate constant for the reaction of CDDT vapor with photochemically generated hydroxyl radicals in the atmosphere has been estimated to be  $1.7 \times 10^{-10}$  cm<sup>3</sup>/molecule-sec at 25°C, which corresponds to a reaction half-life of 0.061 days. The Henry's Law constant for CDDT is estimated to be  $3.48 \times 10^{-3}$  atm-m<sup>3</sup>/mole, and the estimated half-life from a river is 4 hours. Biodegradation is not expected to be an important fate process. Fugacity model predictions indicate that CDDT will partition mainly to the air, with virtually none going to water, soil, or sediment. The reported log Kows for this test substance range from 4.1 to 5.8. Since there is such disparity in log Kow values, a determination of log Kow using the slow-stir-flask method is recommended. The Bioconcentration Factor (BCF) was estimated as 286 to 3428, based on a log Kow measurement of 4.1 to 5.5; therefore, there is a predicted moderate potential for this compound to bioaccumulate. Since BCF and fugacity data were estimated based on log Kow measurements, they may be recalculated when the results of the proposed log Kow test are complete. Bioaccumulation is unlikely to be an issue, however, given the relatively high vapor pressure, water solubility, and low estimated stability of the compound in water. The production and use patterns of the test substance also make bioaccumulation an unlikely issue.

1,5,9-Cyclododecatriene was moderately toxic to fish, slightly toxic to algae, and moderately or highly toxic to *Daphnia* or shrimp, respectively. Based on measured test concentrations, the following endpoint values have been reported: 96-hour LC<sub>50</sub> in sheepshead minnows of 2.02 mg/L, 48-hour EC<sub>50</sub> in *Daphnia* of ca. 5 mg/L, 96-hour LC<sub>50</sub> in shrimp of 0.47 mg/L, and 4-day EC<sub>50</sub> in algae of ca. 140 mg/L.

1,5,9-Cyclododecatriene is slightly toxic via oral and inhalation routes, with an LD<sub>50</sub> and LC<sub>50</sub> in rats of 2500 mg/kg and 8.2 mg/L (1230 ppm), respectively. 1,5,9-Cyclododecatriene has a dermal LD<sub>50</sub> of > 3520 mg/kg. 1,5,9-Cyclododecatriene is a skin and eye irritant. Although the majority of the studies (total of 3) determined that 1,5,9-cyclododecatriene was not a skin sensitizer, one study determined that it was a potent skin sensitizer in animals.

Repeated exposures to 260 ppm of 1,5,9-cyclododecatriene via inhalation produced minimal, reversible effects in the nasal tissue of rats. Histologically, no other evidence of systemic toxicity was observed at this dose level or at 50 ppm. Repeated exposure to 1,5,9-cyclododecatriene produced clinical signs of toxicity (260 ppm) and a decrease in body weights (50 and 260 ppm); however, these changes were reversible. In a repeated dose, developmental/reproductive toxicity screening test, when male rats were dosed with 300 mg/kg 1,5,9-cyclododecatriene via gavage, a test-substance related, biologically significant decrease in

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body weight gains, accompanied by increased food consumption, and decreased food efficiency was observed. Females administered 100 or 300 mg/kg/day had test substance-related, significantly decreased body weight and body weight gain during gestation that was accompanied by a significant increase in food consumption (300 mg/kg/day only) and significantly decreased food efficiency in 100 and 300 mg/kg/day females. There were no other test substance related effects on clinical observations, neurobehavioral parameters, motor activity, clinical pathology, organ weights, or tissue morphology in males or females at 30, 100, or 300 mg/kg 1,5,9-cyclododecatriene. Body weights of pups in the 300 mg/kg/day group were significantly decreased on lactation days 0 and 4. There were no test substance-related effects on clinical observations, number of pups born, number of pups born alive, number of pups surviving through lactation day 4, or reproductive parameters examined. Based on body weights and/or food consumption the no-observed-adverse-effect levels in this screening test (described above) were 100 mg/kg/day for males, 30 mg/kg/day for females, and 100 mg/kg/day for pups. No effects on reproductive parameters were observed.

Female rats were exposed to 0, 10, 25, or 67 ppm 1,5,9-cyclododecatriene on gestation days 6-20. Although maternal toxicity in the rat, evidenced as decreases in body weight and food consumption, and increase in clinical signs was observed at 67 ppm and 25 ppm 1,5,9-cyclododecatriene, developmental toxicity was observed only at 67 ppm. No maternal or developmental toxicity was observed at 10 ppm 1,5,9-cyclododecatriene. The results of this study indicate that 1,5,9-cyclododecatriene is not likely to be uniquely toxic to the rat conceptus.

The compound was negative in the *in vitro* bacterial reverse mutation assay (*Salmonella* and *E. coli*), the *in vitro* clastogenicity study with human lymphocytes, and the *in vivo* rat micronucleus assay.

1,5,9-Cyclododecatriene is manufactured at only one facility, which is located in a rural area in Texas. The majority of the production volume (85%) of the test substance is site limited and used to produce cyclododecane, also a site-limited intermediate, which is used in the production of dodecanedioic acid. The remaining 15% of the production volume is sold to customers who use and consume the substance exclusively as a chemical intermediate. DuPont assesses the capability of a customer using the Product Stewardship System prior to selling a product. The Product Steward works with customers to get an understanding of their application and covers issues pertaining to the use of PPE (personal protective equipment), safety equipment (safety showers, eyewash stations, ventilation needs, etc.), storage concerns, disposal requirements, and any questions concerning the Material Safety Data Sheet.

The single-production facility for the test substance can have as many as 2000 personnel working on-site (construction, contractor, and plant employees), however, the area where the substance is manufactured will have from 2 operators during normal operations up to a total of 60 people during a shutdown or major construction activity. Occupational exposure to 1,5,9-cyclododecatriene is expected to be of low concern when the chemical is handled in accordance with appropriate industrial hygiene and safety measures. Industrial hygiene systems are in place to monitor and assess potential hazards, and implement control measures where needed. The Acceptable Exposure Limit established by DuPont Haskell Laboratory is 2 ppm (13 mg/m<sup>3</sup>) (8- and 12-hour TWA), and measured airborne concentrations in the workplace are

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within the recommended limits. To keep employee exposure below recommended limits, a combination of engineering controls and PPE are required. Adequate safety equipment, such as safety showers, eyewash fountains, and washing facilities are available in the event of an occupational exposure. Individuals handling 1,5,9-cyclododecatriene should avoid contact with eyes, skin, and clothing, thoroughly wash after handling, and avoid breathing any vapors or mist. Workers use impervious clothing and are not required to wear respirators during the routine operation of the plant.

Releases to the environment are expected to be minimal under standard operating conditions. Releases to water are negligible, and approximately 1500 lbs. or less are released to the atmosphere on an annual basis. The C12 Unit emissions are well below fence line limits established by the state of Texas.

**TEST PLAN FOR 1,5,9-CYCLODODECATRIENE**

<b>1,5,9-Cyclododecatriene CAS No. 4904-61-4</b>	<b>Data Available</b>	<b>Data Acceptable</b>	<b>Testing Required</b>
	<b>Y/N</b>	<b>Y/N</b>	<b>Y/N</b>
<b>PHYSICAL/CHEMICAL CHARACTERISTICS</b>			
Melting Point	Y	Y	N
Boiling Point	Y	Y	N
Vapor Pressure	Y	Y	N
Partition Coefficient (log Kow)	Y	N	Y
Water Solubility	Y	Y	N
<b>ENVIRONMENTAL FATE</b>			
Photodegradation	Y	Y	N
Stability in Water	Y	Y	N
Transport (Fugacity)	Y	Y	N
Biodegradation	Y	Y	N
<b>ECOTOXICITY</b>			
Acute Toxicity to Fish	Y	Y	N
Acute Toxicity to Invertebrates	Y	Y	N
Acute Toxicity to Aquatic Plants	Y	Y	N
<b>MAMMALIAN TOXICITY</b>			
Acute Toxicity	Y	Y	N
Repeated Dose Toxicity	Y	Y	N
Developmental Toxicity	Y	Y	N
Reproductive Toxicity	Y	Y	N
Genetic Toxicity Gene Mutations	Y	Y	N
Genetic Toxicity Chromosomal Aberrations	Y	Y	N